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Detection of contaminant plumes released from landfills

N. B. Yenigül¹, A. T. Hendsbergen², A. M. M. Elfeki³, and F. M. Dekking²

¹Delft University of Technology, Faculty of Civil Engineering and Geosciences, Water Resources Section, The Netherlands

²Delft University of Technology, Faculty of Electrical Engineering, Mathematics and Computer Science, The Netherlands

³King Abdulaziz University, Faculty of Meteorology, Environment and Arid Land Agriculture, Department of Hydrology and Water Resources Management, Kingdom of Saudi Arabia

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Correspondence to: N. B. Yenigül (n.b.yenigul@citg.tudelft.nl)

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Abstract

Contaminant leaks released from landfills are a significant threat to groundwater quality. The groundwater detection monitoring systems installed in the vicinity of such facilities are vital. In this study the detection probability of a contaminant plume released from a landfill has been investigated by means of both a simulation and an analytical model for both homogeneous and heterogeneous aquifer conditions. The results of the two models are compared for homogeneous aquifer conditions to illustrate the errors that might be encountered with the simulation model. For heterogeneous aquifer conditions contaminant transport is modelled by an analytical model using effective (macro) dispersivities.

The results of the analysis show that the simulation model gives the concentration values correctly over most of the plume length for homogeneous aquifer conditions, and that the detection probability of a contaminant plume at given monitoring well locations match quite well. For heterogeneous aquifer conditions the approximating analytical model based on effective (macro) dispersivities yields the average concentration distribution satisfactorily. However, it is insufficient in monitoring system design since the discrepancy between the detection probabilities of contaminant plumes at given monitoring well locations computed by the two models is significant, particularly with high dispersivity and heterogeneity.

1 Introduction

Contaminants are introduced in the groundwater by planned human activities rather than natural ones. Landfills, storage and transportation of commercial materials, mining, agricultural operations, interaquifer exchange and saltwater intrusion are the major sources of groundwater contamination. Among these, landfills represent a widespread and significant threat to groundwater quality, human health, and even more to some of the ecosystems. In communal language landfill means waste disposal on land. How-

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ever, technically one may define landfill as “the engineered deposit of waste onto or into land in such a way that pollution or harm to the environment is prevented and through restoration of land provided which may be used for other purpose” (Bagchi, 1994). Unfortunately in many places the environmental impact of landfill leakage, particularly on groundwater quality, has been encountered several times, regardless of an ideal site selection and a thriving design. Works by Mikac et al. (1998), Tatsi and Zouboulis (2002), Chofqi et al. (2004) are only few of countless examples presented in the literature. The risk of groundwater contamination can be further reduced by monitoring its quality via a monitoring system composed of a series of wells located around the landfill and sampled periodically for contaminants. However, it is difficult to ensure that a specific monitoring system will detect all of the contaminants released from the landfill because of the numerous and significant uncertainties involved. Size and location of the possible contaminant leak, spatial variability of the hydrogeological characteristics (which make groundwater flow and contaminant paths hard to predict), locations, depth and number of monitoring wells, chemical characteristics of contaminants and sampling procedure are the source of uncertainties that have great influence on the detection probability of contaminant plumes, or in other words, the efficiency of a monitoring system.

Several studies on the monitoring problem have been presented in the literature. Most of these studies do not incorporate all the relevant factors due to the complexity of the issue. In general the approaches based on geostatistical methods (i.e. Rouhani and Hall, 1988; Haugh et al., 1989), optimization methods (i.e. Hudak and Loaiciga, 1993; Meyer et al., 1994; Storck et al., 1997), methods based on extensive simulation (Massmann and Freeze, 1987; Meyer et al., 1994; Storck et al., 1997) and graphical methods (Hudak, 2001 and 2002) are used to design monitoring systems.

In this study the detection probability of a contaminant plume released from a landfill has been investigated by means of both a simulation and an analytical model. Analytical models are generally available only for very simplified situations such as homogeneous medium and uniform flow. Simulations are used to incorporate the properties

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related to heterogeneity, as geologic environments are seldom uniform and homogeneous. The assumption of homogeneous conditions (e.g. hydraulic conductivity constant in space) in groundwater flow problems may yield an appropriate approximation in some situations. In contamination problems however, the extent and characteristics of a contaminant plume may be significantly influenced by the heterogeneous nature of geologic formations. Areas of low hydraulic conductivity may slow the flow and reduce the spreading of a plume, whereas high conductivity zones may cause channelling of the plume and abrupt changes in contaminant concentrations. These types of regimes cannot be appropriately analyzed under assumptions of a homogeneous medium. Still, the significance of analytical models should not be underestimated, as they are important tools to verify the simulations and to obtain a thorough understanding of the phenomena. Hence in the first part of the paper, homogeneous aquifer conditions are considered. The concentration distribution of contaminants and the detection probability of monitoring wells are determined for both instantaneous and continuous leak cases by simulation and analytical models. The results of the simulation model are compared with those of the analytical model for homogeneous aquifer conditions to illustrate the errors that might be encountered with the simulation model and to investigate the influence of certain parameters.

In the second part of the paper, a comparison between results of simulations and results of a particular analytical model in heterogeneous aquifer conditions is presented. Since there is a general agreement that hydraulic conductivity variations play an important role in contaminant transport a very primitive worst case assumption for homogenization of a heterogeneous medium might be using a large hydraulic conductivity value (although still homogeneous). This may result in over estimation of the velocity and extent of the plume. Consequently, this may result in very conservative and costly monitoring. On the other hand, if a very small value of hydraulic conductivity is used, unconservative designs may result in under estimation of the contaminant plume. In the last two decades a significant amount of research has been devoted to the comprehension of the effects of natural heterogeneity on solute transport and to the

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development of modelling techniques which explicitly account for natural heterogeneity (e.g. Gelhar et al., 1979; Gelhar and Axness, 1983; Dagan, 1984, 1986; Vomvoris and Gelhar, 1990; Thompson and Gelhar, 1990; Rubin, 1990; Kapoor and Gelhar, 1994a, b; McLaughlin and Ruan, 2001; Hu et al., 2002; etc.). Clearly, modelling of contaminant transport using an advection-dispersion equation with effective (macro) dispersivities is common practice. The effective (macro) dispersion coefficient embodies the effect of unresolved advective heterogeneity on the spatial second moment and can be used to describe the average concentration distribution. In this study, the mean concentration field is determined (e.g. Kapoor and Gelhar, 1994) using the effective dispersion coefficient in the analytical model. Here the effective dispersion coefficient is the summation of the local dispersivities and constant macrodispersivities as computed by Gelhar and Axness, 1983 and the detection probability of the contaminant plume is computed for homogenized heterogeneous aquifer conditions. The results of the analysis based on the simulation and analytical model are compared to find the answers to the questions: How far an analytical model can be used in groundwater monitoring system design while incorporating the effects of various heterogeneities on contaminant transport? How accurate can the detection probability of a contaminant plume by a given monitoring well be computed by an analytical model, which uses macrodispersivities to homogenize the heterogeneity? How large will be the discrepancies between the results obtained by the two models?

2 Description of the simulation model

A Monte Carlo approach coupled with a two dimensional finite difference flow model and a random walk particle-tracking model (adapted from Elfeki, 1996) is used to simulate a large number of contaminant plumes released from a landfill. The heterogeneity of the subsurface and the leak locations are the uncertainties incorporated in the simulation model.

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2.1 Two dimensional groundwater flow model

A two dimensional model of steady-state saturated groundwater flow in an isotropic heterogeneous aquifer is applied on a rectangular domain of dimension ($0 \leq x \leq L_x$, $0 \leq y \leq L_y$). The equation to be solved is

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) = 0 \quad (1)$$

where K_{xx} is the hydraulic conductivity in the x -direction [L/T], K_{yy} is the hydraulic conductivity in the y -direction [L/T] and h is the hydraulic head [L]. A block-centered five-point finite difference method is used to discretize Eq. (1). Dirichlet and Neumann boundary conditions are considered. The conjugate method is used to solve the symmetric system of equations. The internodal Darcy's velocity components are computed once the hydraulic head is obtained as a function of and at the centre of each grid cell. Then, the average groundwater flow velocities in the x -direction (v_x) and y -direction (v_y) are calculated by dividing the Darcy velocities by the effective porosity of the medium.

2.2 Particle tracking model for contaminant transport

In this study the movement of contaminants in the subsurface is represented by the advection-dispersion equation. The contaminant is assumed to be conservative and to have no interaction with the solid matrix. A transient plume migration in a steady state flow domain is considered. The two-dimensional advection-dispersion equation for this case can be written as (Bear, 1972):

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} - \frac{\partial}{\partial x} \left[D_{xx} \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y} \right] - \frac{\partial}{\partial y} \left[D_{yx} \frac{\partial C}{\partial x} + D_{yy} \frac{\partial C}{\partial y} \right] = 0 \quad (2)$$

where C is the concentration of the contaminant at time t at location (x, y) , v_x and v_y are the average groundwater flow velocity components in the x - and y -direction respectively, and D_{xx} , D_{xy} , D_{yx} , D_{yy} are the components of the pore scale hydrodynamic

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dispersion tensor. Having obtained the velocity field for each realization of the hydraulic conductivity field, the solution of the transport equation and the spatio-temporal evolution of the concentration field are obtained by employing a random walk particle model. It is assumed that $C(x, y, 0) = 0$ for $0 \leq x \leq L_x$, $0 \leq y \leq L_y$. The boundary condition

5 $\partial C / \partial y(x, 0, t) = 0$, $\partial C / \partial y(x, L_y, t) = 0$ for $t \geq 0$ is imposed. The contaminant source is located at the upstream side of the model domain.

In this study the random walk particle tracking model is used to incorporate dispersion since it facilitates the solution of problems having zero or low dispersivity values (large Peclet numbers), and since it does not exhibit numerical dispersion (Kinzelbach, 10 1986). The injected contaminant mass is represented by particles moving in the flow field. Each particle is assigned the same fixed amount of contaminant mass. Dispersion is modelled by superimposing a random movement on the convective particle movement, which has the statistical properties that correspond to the properties of the physical dispersive process. A large number of individual random walks of particles 15 form a dispersing particle cloud characterizing a contaminant mass distribution.

In the random walk particle tracking model the concentration distribution at a fixed time has the form of the probability density function of a normal variable with mean value μ and standard deviation of σ :

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (3)$$

20 The solution to the advection-dispersion equation in one dimensional form for an instantaneous release of a solute of M_0 from location x_0 , longitudinal dispersivity α_L , and mean groundwater flow velocity v_x in the x -direction, is:

$$C(x, t) = \frac{C_0}{\sqrt{4\pi\alpha_L v_x t}} \exp \left[-\frac{(x - x_0 - v_x t)^2}{4\alpha_L v_x t} \right] \quad (4)$$

where $C_0 = M_0 / \varepsilon H$, with the effective porosity and the aquifer thickness.

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Comparing the two equations, it is clear that the mean value and the standard deviation are:

$$\mu = x_0 + v_x t \quad (5)$$

$$\sigma = \sqrt{2\alpha_L v_x t} \quad (6)$$

- 5 implying that the position of the centre of the plume moves at the groundwater velocity and the plume disperses around this centre with a standard deviation that depends on the dispersion coefficient and increases linearly with time.

Given the analogy between the transport equation (Eq. 2) and the Fokker-Planck equation (Uffink, 1990), the two-dimensional particle tracking equations incorporating
10 dispersion can be written as (Kinzelbach, 1986):

$$X_p(t+\Delta t) = X_p(t) + v_x \Delta t + \left(\frac{\partial D_{xx}}{\partial x} + \frac{\partial D_{xy}}{\partial y} \right) \Delta t + \frac{v_x}{|v|} Z \sqrt{2\alpha_L |v| \Delta t} - \frac{v_y}{|v|} Z' \sqrt{2\alpha_T |v| \Delta t} \quad (7)$$

$$Y_p(t+\Delta t) = Y_p(t) + v_y \Delta t + \left(\frac{\partial D_{yx}}{\partial x} + \frac{\partial D_{yy}}{\partial y} \right) \Delta t + \frac{v_y}{|v|} Z \sqrt{2\alpha_L |v| \Delta t} + \frac{v_x}{|v|} Z' \sqrt{2\alpha_T |v| \Delta t} \quad (8)$$

- where $X_p(t)$, $Y_p(t)$ are the x- and y-coordinates of a particle at time t , is the time step used in calculations, Z , Z' are two independent random numbers drawn from a
15 normal distribution with mean zero and variance one, α_L is the longitudinal, and α_T the transverse dispersivity and v is the resultant flow velocity.

On the right hand sides of both Eqs. (7) and (8), the first terms correspond to the previous position of the particle, the second terms correspond to the convective displacement, the third terms are the Fokker-Plank term (a counter-term has to be added
20 to correct the unrealistic accumulation of particles at stagnation zones), and the last two terms are the stochastic dispersive displacements projected in the x- and the y-directions respectively.

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The solution of the advection-dispersion transport equation by the random walk method provides the discrete particle displacements and not the concentration values. A discretized grid model, similar to the one used in the solution of groundwater flow equations, is superimposed to convert the particle displacements into concentrations.

- 5 The average concentration at time t in a grid cell (i, j) with dimensions Δx and Δy in (x - and y -directions respectively), is:

$$C_{ij}(t) = \frac{M_o n_{ij}(t)}{N \varepsilon d_{ij} \Delta x \Delta y} \quad (9)$$

- where $C_{ij}(t)$ is the volume averaged concentration in grid cell (i, j) at time t , $n_{ij}(t)$ is the number of particles in grid cell (i, j) at time t , N is the total number of particles released and d_{ij} , is the thickness of the grid cell, which is considered as unit thickness in this study (2D model).

- One should be aware that the number of particles used in the model has a great influence on the computation of concentration values. In advection modelling, two particles at the same initial location will follow the same path since it is only determined by the groundwater flow field; hence a small number of particles is needed, which reduces the computational effort. On the other hand, when modelling dispersion, the number of particles used is very important. Since spreading of the contaminants is affected by a random component, two particles placed at the same initial location will most likely follow different paths, although on average (due to the law of large numbers) they will follow the advective transport path. A small number of particles may not model the spreading of the plume appropriately, resulting in incorrect estimates of the contaminant concentration.

- In addition, the time and release rate of contaminants will influence the concentration characteristics. For the simulation of a continuous leak, new particles start from the source location at every time step. This is computationally very expensive since it leads to the use of a very large number of particles. However in the case of a stationary flow field and a source of constant strength a continuous source can be simulated

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by convolution from the solution for an instantaneous pulse of contaminants using a relatively small number of particles (Kinzelbach, 1986). It is assumed that particles released at time will follow the same paths as particles released at t . The concentration distribution in every time step is obtained by adding the moving particles to the old concentration distribution.

2.3 Probability of detection

A Monte Carlo simulation procedure is used to compute the detection probability, $P_{d(mw)}$ of a given monitoring well. First, a realization of a random hydraulic conductivity field (for heterogeneous media) is generated. After solving the steady state groundwater flow model to determine the velocity field a random leak location is generated. Then the random walk transport model is solved to determine the concentration field of the contaminant plume until it reaches the compliance boundary. Finally, the model checks whether the concentration value at a given monitoring well location exceeds a given threshold concentration (detection limit) to determine whether a plume is detected or not detected by a given monitoring well.

Detection of a contaminant plume by a monitoring well (mw), is defined as the event where the contaminant concentration at the well location, C_{mw} at some time t is equal to or greater than a given threshold concentration C_{TH} . Therefore the probability of detection $P_{d(mw)}$ of a given plume by a given monitoring well is:

$$P_{d(mw)} = P(C_{mw} \geq C_{TH}, \text{ at some time } t) = \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} I_d^{(i)} \quad (10)$$

Here, N_{MC} is the total number of simulation runs, i.e. the number of the plumes, $I_d^{(i)}$ is the indicator function of detection by the monitoring system for realization i , i.e. $I_d^{(i)}$ equals 1 if the simulated contaminant plume i is detected by the given monitoring well, and equals zero otherwise.

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3 Description of the analytical model

3.1 Homogeneous aquifer conditions

The concentration at position (x, y) and at time t due to an instantaneous release of contaminant at location (x_0, y_0) is given by (Bear, 1972),

$$C(x, y, t) = \frac{C_0}{\sqrt{4\pi\alpha_L v_x t} \sqrt{4\pi\alpha_T v_x t}} \exp - \left[\frac{(x - x_0 - v_x t)^2}{4\alpha_L v_x t} + \frac{(y - y_0)^2}{4\alpha_T v_x t} \right] \quad (11)$$

This is a pointwise, concentration whereas in the simulation model the concentration is calculated by means of particles in a grid cell (see Eq. 9). Hence one must average the concentration over the grid cells in order to make an equitable comparison between the concentration values calculated by the analytical and the simulation model. Therefore a weighted average of the theoretical concentration with weights corresponding to Simpson's rule for dimension 2 is used in the analytical model. In highly dispersive media and/or far away from the source the averaging does not make much difference since the plumes are already quite spread out in such cases. However for the locations where the plume is very peaked the effect will be very noticeable. But even in the region where the averaging does not matter, the Simpson approximation for the integral over a grid cell will give a small bias.

To find the concentration of a plume resulting from a continuous leak two different approaches can be taken. The first approach is to approximate such a plume by repeated small instantaneous plumes at short time intervals. In fact, taking the intermittent time intervals shorter and shorter, apart from inherent numerical instability around the origin, in this way the exact concentration will be approached better and better. The second approach is to use the approximation of the concentration by the Hantush well function (Kinzelbach, 1986). Calculations with Matlab showed that for wells not too far from the source the two approximations are quite close, but further away the Hantush approximation breaks down. The Hantush function looks like an elegant closed form, but the

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improper integral it contains limits its numerical application. For large x-values, numerical breakdown occurs as in the Hantush formula a very large number is multiplied with a number close to zero.

3.2 Heterogeneous aquifer conditions

- 5 Heterogeneity can be dealt with by defining the homogeneous equivalent properties, known as averaging. The advection-dispersion equation that includes the effect of the variations of velocities at the local and regional scale on solute dispersion to describe the (average) solute transport can be written as (Kapoor and Gelhar, 1994):

$$\frac{\partial \bar{C}}{\partial t} + v \frac{\partial \bar{C}}{\partial x_1} - v(A_{ij} + \alpha_{ij}) \frac{\partial^2 \bar{C}}{\partial x_i \partial x_j} = 0 \quad (12)$$

- 10 where \bar{C} is the mean concentration, v is the mean velocity in the x_1 direction, A_{ij} and α_{ij} are the macrodispersivities and local dispersivities, respectively. The mean concentration, governed by Eq. (12) for an instantaneous release of contaminant is assumed to be Gaussian. Thus in order to include both local and regional dispersion in the analytical model and compute the mean concentration value at position (x, y) and time t due to an instantaneous release of contaminant at location (x_0, y_0) (Eq. 11) is modified as follows:

$$\bar{C}(x, y, t) = \frac{C_0}{\sqrt{4\pi(A_L + \alpha_L)v_x t} \sqrt{4\pi(A_T + \alpha_T)v_x t}} \exp - \left[\frac{(x - x_0 - v_x t)^2}{4(A_L + \alpha_L)v_x t} + \frac{(y - y_0)^2}{4(A_T + \alpha_T)v_x t} \right] \quad (13)$$

Theoretically derived A_L and A_T values are given by (Gelhar and Axness, 1983),

$$A_L = \sigma_Y^2 \lambda / \gamma^2 \text{ and } A_T = \frac{\sigma_Y^2 \alpha_L}{8\gamma^2} \left(1 + 3 \frac{\alpha_T}{\alpha_L} \right) \quad (14)$$

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where λ and σ_Y are the correlation length and standard deviation of the $\ln K$ field. γ is a flow factor, which for the isotropic case is $\gamma=1+\sigma_Y^2/6$ and $\gamma \simeq 1$ if it is assumed that the local dispersivity α_L is small compared to correlation length λ . In this study γ is considered to be 1 since α_L is taken in the order of centimeters, while λ is in the order of meters.

Similar to the homogeneous aquifer conditions, from a continuous leak such a plume is approximated by repeated small instantaneous plumes at short time intervals to find the mean concentration distribution as the mean groundwater velocity and injection rate are considered to be constant (Vomvoris and Gelhar, 1990). For both instantaneous and continuous leak cases, the mean concentration values will be used to determine the detection probability of a contaminant plume by a given monitoring system.

3.3 Probability of detection

Plumes start from a random location (x_0, y_0) where x_0 is fixed and y_0 is between y_c-L and y_c+L where $2L$ is the length of the landfill. Detection of such a plume by a well located at position (x_{mw}, y_{mw}) occurs if the concentration at the monitoring well $C(x_{mw}, y_{mw}, t)$ is greater than or equal to the threshold concentration C_{TH} at some moment in time. By calculating the maximum concentrations on the line $x=x_{mw}$ the maximum width of the plume, (above a given threshold) at x_{mw} can be found (See Appendix A).

Define the detection region $D(x_0, y_0, C_{TH})$ as the set of the points (x, y) where at some moment in time a plume starting from (x_0, y_0) will be detected at level C_{TH} . Likewise let the leak-region $L(x_{mw}, y_{mw}, C_{TH})$ be the set of points (x, y) such that a plume starting from (x, y) will be detected by a well at location (x_{mw}, y_{mw}) . In a homogeneous medium the shape of a plume is the same whatever its starting point and the leak region and the detection region for one and the same point (x, y) are each other's image under reflection in the point (x, y) (see Fig. 1). Suppose that the plume released from (x_0, y_0) has width $2l$ at distance x_{mw} from the source. Any leak on the line $x=x_0$ between $y_{mw}-l$ and $y_{mw}+l$ will be detected; any leaks with other y -values will not. The detec-

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tion probability is thus simply the fraction of the line segment $x=x_0$, $y_c-L \leq y \leq y_c+L$ that is covered by $[y_{mw}-l, y_{mw}+l]$. As long as $l < L$ and $[y_{mw}-l, y_{mw}+l]$ falls completely within $[y_c-L, y_c+L]$, which happens if $y_c-L+l \leq y_{mw} \leq y_c+L-l$, the detection probability is therefore

$$P_{d(mw)} = \frac{2l}{2L} = \frac{l}{L}. \quad (15)$$

When calculating the detection probability of a well close to the boundaries or when $L \leq l \leq 2L$ a boundary effect should be taken into account (see Appendix B). Last of all, if $l > 2L$ then any leak within $[y_c-L, y_c+L]$ will be detected.

4 Illustrative example

The model domain is of size $L_x=500$ m and $L_y=400$ m (Fig. 2). The model is discretized with grid cells of 2 m by 2 m in both x -direction and y -direction. The hypothetical landfill is located at $30 \leq x \leq 50$ m and $180 \leq y \leq 220$ m in the model domain. The monitoring wells are located in the rectangle $60 \leq x \leq 450$ m and $180 \leq y \leq 220$ m. In order to achieve a detailed comparison between the analytical and the simulation model in terms of estimated concentrations and detection probability values the distance between the monitoring wells is set to 10 m (5 grid cells) in the x -direction and 2 m in the y -direction.

The boundary conditions for the groundwater flow are: zero flux at $y=0$ m (bottom boundary) and $y=400$ m (top boundary) and constant head along the left and the right boundaries. The head values at $x=0$ m and $x=500$ m were chosen to result in a macroscopically constant hydraulic gradient of 0.001. Porosity equals 0.25. The average hydraulic conductivity K is set to 10 m/day and for homogeneous aquifer conditions the location of the leak is the only random input to the model.

For the heterogeneous aquifer, uncertainties due to both the contaminant source location and the subsurface heterogeneity are incorporated in the simulation model. Subsurface heterogeneity is reflected by the spatial variability of the hydraulic conductivity. Hence hydraulic conductivity is treated as a random space function or random

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field. The logarithm of the isotropic hydraulic conductivity $Y=\ln(K)$ is modelled as a stationary Gaussian field with a given mean, variance and correlation length (see e.g. Gelhar, 1986).

Random conductivity fields that respect these statistics are generated using the turning bands method (Mantoglou and Wilson, 1982). The value of μ_Y is set to 2.3, whereas the variance of Y , σ_Y^2 , is assigned four different values, namely 0.2, 0.4, 1.0 and 1.5, respectively. The value of $\mu_Y=2.3$ corresponds to a geometric mean of the hydraulic conductivity of 10 m/day. The isotropic covariance of Y is chosen to be of exponential form with a correlation length $\lambda=15$ m.

For the transport model a condition of a zero dispersive flux is imposed on the top and bottom boundary, and the initial background concentration in the model domain is set to zero. Since the flow direction is parallel to the x -axis, the only source dimension that is treated as a random variable is its y -coordinate. Potential leak locations occur along the downgradient edge of the landfill. The contaminant leak is assumed to be a point source, as it would result in a plume, which is most difficult to detect, and the source location is drawn from a uniform probability distribution between y -coordinates of $180 \leq y \leq 220$ m for each Monte Carlo run. Calculations are carried out for two types of leak, namely instantaneous and continuous leaks. The initial concentration for the instantaneous leak is assumed to be 1 mg/l whereas for the continuous the leak case injection rate is set to 1 mg/l/day. The threshold concentration (detection limit) at which detection occurs is set at 0.5% of the initial source concentration. Contaminants are assumed to be conservative and to be completely mixed over the depth of the aquifer. Dispersion is incorporated in the model by introducing microscale longitudinal (α_L) and transversal (α_T) dispersivity. The ratio between α_L and α_T is assumed to be 10, (Bear, 1972). α_L is set to 0.1 m and 0.5 m. Since a two-dimensional model is used in this study it is assumed that the monitoring wells are fully penetrating the aquifer, and that they are located in the centres of the grid cells, having a dimension of one grid cell. It is supposed that sampling is continuous.

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5 Results and discussion

5.1 Assessment of simulations by analytical methods for the homogeneous case

In order to investigate the accuracy of the simulation model and the influence of the parameters on estimated values, the solution of the simulation model is compared to the results obtained by the analytical model.

5.1.1 Instantaneous leak

For plume simulations 500, 1000, 2000, 4000 and 8000 particles are used in order to investigate the influence of the number of particles on the computation of concentration values and to determine the appropriate number of particles to be used throughout the computations.

The simulations are performed for the cases where, $\alpha_L=0.1$ m, $\alpha_T=0.01$ m and $\alpha_L=0.5$ m, $\alpha_T=0.05$ m respectively. In both cases the plumes originate from an instantaneous leak at the fixed location $x=50$ m and $y=200$ m. Figure 3 shows the different longitudinal sections of simulated plumes and comparison with the analytical solution for $\alpha_L=0.1$ m, $\alpha_T=0.01$ m. As is seen in the figure the differences between the plume simulations with 500, 1000, 2000, 4000 and 8000 particles are minor. Nevertheless, the plume edge (which occurs around $y=204$ m) is defined the worst by 500 particles and the best by 8000 particles. The same trend is also observed for $\alpha_L=0.5$ m, $\alpha_T=0.05$ m. Since simulations of 8000 particles are computationally very expensive, 2000 particles are used in the rest of the analysis, as a compromise value.

The concentration values obtained by simulations are quite accurate over most of the plume length. However, near the source there is a slight discrepancy between the simulation and analytical models especially when the dispersivity value is low. The plumes are narrow close to the source and widen as they move away. Therefore close to the source the concentration values determined by the analytical model are more peaked. The averaging of the analytical solution over a grid cell using Simpson's Rule

will then overestimate the average concentration. This also leads to higher discrepancy between the two models in the low dispersive medium ($\alpha_L=0.1$ m, $\alpha_T=0.01$ m, shown in Fig. 3) compared to the highly dispersive medium ($\alpha_L=0.5$ m, $\alpha_T=0.05$ m, not shown).

Figure 4 shows the comparison of the detection probabilities computed by the simulation and the analytical model at the selected well locations for both dispersivity cases. The possible leak locations are now randomly located at $x=50$ m and over $180 \leq y \leq 220$ m. The values estimated by the simulation model are compatible with those estimated by the analytical model. The slight discrepancy seen in the graphs is due to the fact that the plume edges are not as sharply defined as in the analytical model.

5.1.2 Continuous leak

Plumes originated from a continuous leak located at $x=50$ m and $y=200$ m with an injection rate of 1 mg/l/day. As in the instantaneous leak case the simulation model estimated the concentration values correctly over the most of the plume length (see Fig. 5). As described above, the slight discrepancy between the simulation and analytical model estimations close to the source, particularly in the low dispersive case, is due to the slender nature of the plume when it is close to the source. The results are representative for the case where $\alpha_L=0.5$ m, $\alpha_T=0.05$ m as well. Figures 6 and 7 present the detection probabilities at selected monitoring wells for continuous leak condition in the homogeneous case for $\alpha_L=0.1$ m, $\alpha_T=0.01$ m and $\alpha_L=0.5$ m, $\alpha_T=0.05$ m, respectively. The possible leak locations are at $x=50$ m and $180 \leq y \leq 220$ m. As seen from the figures the discrepancy between the analytical and simulation model estimations is much less than in the instantaneous case. This is mainly due to the fact that the convolution procedure described at the end of Sect. 2.2 yields better approximations of the plume with less particles than in the instantaneous leak case.

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5.2 Assessment of simulations by analytical methods for the heterogeneous case

The results of the analytical model described in Sect. 3.2 and the simulation model described in Sect. 2.2 are expressed in terms of concentration profiles along the specified longitudinal sections and plots of the detection probability as a function of the distance from the contaminant source to determine: (1) how good is the mean concentration as a predictor of the concentration at a given monitoring well location, and (2) how accurate is it to use the mean concentration value in computing the detection probability of a contaminant plume by a given well in a sample realization of the hydraulic conductivity field. The computations are carried out for eight different scenarios. Table 1 summarizes the parameters for all cases.

5.2.1 Instantaneous leak

The actual concentration field is observed in a single heterogeneous aquifer and should be viewed as a realization of the stochastic process, whereas the ensemble mean represents the average behaviour of solute plumes in a large number of statistically identical aquifers. The observed concentration distribution does not form a smooth curve, as the mean concentration would, but is quite irregular. Hence the ensemble mean value is not sufficient for the description or prediction of the actual concentration distribution and a successful prediction should be made in a probabilistic context (in terms of predictions accompanied by a quantification of the deviation around the mean values) rather than in the traditional deterministic framework (in terms of mean concentration only). Figure 8 presents the concentration values at given monitoring well locations for three different single realizations, the ensemble mean concentration over 700 simulations and their 95% (empirical) confidence interval along with mean concentration values computed by the analytical model for Case 1a and Case 2d. Case 1a represents the lowest while Case 2d represents the highest dispersive and heterogeneous medium among the scenarios considered in this study. The analysis results corresponding to these cases characterize the others as well. As before the instan-

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taneous leak is located at $x=50\text{ m}$ and $y=200\text{ m}$ in order to compare concentration profiles while random leaks at $x=50\text{ m}$ and along $180\leq y\leq 220\text{ m}$ are taken to compare the detection probabilities.

The average concentration values computed by the two models are close to each other and present a smooth curve compared to single realizations. Concentration values of the single realizations are relatively scattered as expected, since each realization shows a different plume velocity and a different spreading. The 95% confidence interval is wider close to the source: in all cases uncertainty in concentration prediction decreases with distance from the source. The ensemble standard deviation in the concentration is higher near the source and reduces significantly as plume moves further away. Near the source the plume is narrow and has a large degree of freedom to spread in different forms from one realization to another. However, further away from the source the plume widens and since it covers a larger area the degree of freedom to spread is not that high and uncertainty is less. Near the source the concentration gradient is high and consequently the uncertainty is high (see Gelhar, 1993). The 95% confidence interval is narrower towards the edge of the plume ($y=204\text{ m}$) for the same reason. The discrepancy between the two models is overall more pronounced in the low dispersive medium.

Figure 9 shows the comparison of the detection probabilities for four of the eight cases- the cases not shown are similar to Case 1a respectively Case 2a. A discrepancy occurs between the analytical and simulation model, particularly close to the contaminant source. The discrepancy between the detection probability values at given well locations tends to reduce as the distance from the source increases.

The analytical model using effective (macro) dispersivities computes the mean concentration distribution, which corresponds to smoother and relatively wider plumes, consequently a much more diluted plume in the case of an instantaneous leak. This results in lower detection probability values than those obtained by the simulation model. In the simulation model each realization views the possible actual plume observed in a single heterogeneous aquifer, and the detection probability at a given well location

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is computed accordingly. The influence of homogenization in terms of underestimating the plume size is more pronounced when the values of the dispersivity and/or σ_Y^2 increases. As an increase in both values adds to the macro dispersivities used in the analytical model, the average plume, which embodies the behaviour of the plume in a heterogeneous medium, becomes larger and consequently yields lower concentration values at the wells (see Eqs. 13 and 14).

5.2.2 Continuous leak

Computations are performed for all cases mentioned in Table 1 for the continuous leak case as well, since this type of leaks is mostly considered in monitoring system design at landfill sites unless there are specific data for the type of the leak. Figure 10 presents the comparison of concentration profiles computed by the two models in the case of a continuous leak with an injection rate of 1 mg/l/day for Case 1a and Case 2d. The other cases are not shown here as these two cases characterize their behaviour well enough.

The discrepancy between the average concentration values computed by the two models decreases as the dispersivity of the medium increases since the plume gets wider and the concentration gradient is smaller for larger dispersivity values. As described above for the instantaneous leak case the 95% confidence interval is wider close to the source and narrower towards the edge of the plume ($y=208$ m) in the continuous leak case as well, since the concentration gradient decreases as the distance from the source increases. However, in this case the influence of heterogeneity is more visible compared to the instantaneous leak case: the confidence interval close to the source appears to be wider when σ_Y^2 increases. This is due to the fact that in the instantaneous leak case the Gaussian plumes spread faster when the heterogeneity and dispersivity of the medium increases and accordingly the concentration values and hence concentration gradient is smaller.

However in the case of a continuous leak the continuous injection of contaminants results in higher concentration values and therefore a larger concentration gradient,

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which actually reflects the apparent influence of heterogeneity: the uncertainty in concentration prediction increases as the degree of heterogeneity increases. This also explains why the discrepancy between average concentration values computed by the two models is higher than in the instantaneous case.

The plume described by the analytical model using effective (macro) dispersivities is an average plume or actually an envelope of possible plumes in many single heterogeneous media, therefore it is larger and smoother and overlooks the behaviour of irregular contaminant spreading on a macro scale, particularly when the concentration gradient is high. Furthermore, the large average plume with high concentration gradient leads the analytical model to overestimate the concentration values at given well locations. Eventually the results show that in any case the dispersivity of the medium (both pore scale and macro scale) is the most important parameter, which dominates the spreading of the plume, and hence the uncertainty in predictions of concentration values.

The detection probability of monitoring wells at a given location as a function of the distance from the source is presented in Figs. 11 and 12 for the continuous leak case in a heterogeneous medium. The potential random leaks are assumed to occur along the downgradient edge ($x=50$ m and $180 \leq y \leq 220$ m) of the landfill as depicted in Fig. 2. There is a big discrepancy between the detection probability values computed by the two models. The reason for that is as explained above: the overestimation of concentration values computed by the analytical model and hence the overestimation of detection probabilities. Therefore as seen in Figs. 11 and 12 the detection probability of monitoring wells at given locations increases as the heterogeneity increases in contrast to the results of the simulation model. The results of the analysis by the simulation model show that the more heterogeneous the medium is, the less the chance is to detect a contaminant plume at a given monitoring well location. The reason for this is that the plumes become more irregular in shape as the uncertainty in flow paths increases. This result of the simulation model is consistent with other previous studies as well (e.g. Massmann and Freeze, 1987; Meyer et al., 1994; Storck et al., 1997, etc.).

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Simulation and analytical models are used to compute concentration distributions and detection probability values at given monitoring well locations. The results of the analysis show that the simulation model estimates the concentration values correctly over most of the plume length for homogeneous aquifer conditions. A slight discrepancy between the two models near the source is due to the fact that the plumes are narrow close to the source and widen as they move away. Therefore close to the source the concentration values determined by the analytical model are more peaked than those determined by the simulation model. An important point is that the accuracy of the estimates by the simulation model is highly dependent on the number of the particles used in the model.

In the homogeneous case, particularly for the continuous leak, the comparison of the results in terms of detection probability match quite well.

As an analytical model for the concentration distributions of a contaminant plume for heterogeneous aquifer conditions, effective (macro) dispersion coefficients are used to solve the advective-dispersive transport equation. A discrepancy between the mean concentration values computed by the two models is observed, particularly in the continuous leak case. The mean concentration plume that results from such an approximation is smooth due to loss of the detailed advective heterogeneity. This reflects in an overlook in the determination of the concentration field and consequently in the computation of the detection probability of a contaminant plume by a given monitoring well. The 95% confidence intervals drawn from the simulations show that the uncertainty in concentration predictions decreases with the distance from the source. The ensemble standard deviation of the concentration is higher near the source and reduces as the plume moves further away. Near the source the plume is narrow and has a large degree of freedom to spread in different forms from one realization to another. However, further away from the source the plume widens and since it covers a larger area the degree of freedom to spread in one realization to another is not that high and uncertainty

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is less. Near the source the concentration gradient is high and consequently the uncertainty is high (see e.g. Gelhar, 1993). Furthermore, the uncertainty in concentration predictions increases as heterogeneity and/or dispersivity of the medium increases.

The results show that modelling of contaminant transport using an advection-dispersion equation with effective (macro) dispersivities can be used to describe the average concentration distribution, but this approach is insufficient in monitoring system design when incorporating the subsurface heterogeneity. The discrepancy between the detection probabilities of contaminant plumes at given monitoring well locations computed by the two models is significant, particularly when the dispersivity and heterogeneity of the medium increase. Therefore, despite the computational expenses, the simulation model is more appropriate for monitoring system design under conditions of heterogeneity.

Appendix A Determining the plume width at fixed well distance

The (vertical) width of the plume at time t at a well distance x_{mw} can be found by solving $C(x_{mw}, y, t) = C_{TH}$ for y which gives,

$$y^2 = 4\alpha_T v_x t \left[\ln \left(\frac{C_0}{C_{TH}} \frac{1}{4\pi \sqrt{\alpha_L \alpha_T} v_x t} \right) - \frac{(x_{mw} - v_x t)^2}{4\alpha_L v_x t} \right] \quad (A1)$$

Define the abbreviation

$$A := \frac{C_0}{C_{TH} 4\pi \sqrt{\alpha_L \alpha_T}} \quad (A2)$$

This gives

$$y = g(t) = \sqrt{4\alpha_T v_x t (\ln A - \ln v_x t) - \frac{\alpha_T}{\alpha_L} (x_{mw} - v_x t)^2} \quad (A3)$$

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To find the maximum $I(I=g(t_{\max}))$, differentiate g with respect to t : one has to solve $g'(t)=0$. This is not analytically feasible. Note that, for fixed t , the contours $C(x, y, t)=\text{constant}$ are ellipses. One would expect the plume has its maximal width at distance x_{mw} when the centre of this ellipse is at x_{mw} , which happens at $t=x_{mw}/v_x$.

Using numerical approximations it is found that the width of the plume for this t is very close to the optimal width. This is the way the maximal width $2l$ of the plume is calculated in the analytical model.

Appendix B Corrections for boundary effects

Here we calculate the corrections to Eq. (14). If $l \leq L$ and, say $y_w + l \geq y_c + L$, the leaks in $[y_c + L, y_w + l]$, which is an interval of length $(y_w + l - y_c - L)$ should not be counted and,

$$P_{d(mw)} = \frac{2l - ((y_w + l) - (y_c + L))}{2L} = \frac{l + L - y_w + y_c}{2L} \quad (\text{B1})$$

Likewise if $y_w - l \leq y_c - L$ then the detection probability equals:

$$P_{d(mw)} = \frac{2l - ((y_c - L) - (y_w - l))}{2L} = \frac{l + L - y_c + y_w}{2L} \quad (\text{B2})$$

If $L \leq l \leq 2L$ and, if $L - l \leq y_w - y_c \leq l - L$ the detection probability P_d equals 1. But if $y_w - y_c \leq L - l$ then the detection probability equals:

$$P_{d(mw)} = \frac{(y_w + l) - (y_c - L)}{2L} = \frac{L + l + y_w - y_c}{2L} \quad (\text{B3})$$

Likewise if $l - L \leq y_w - y_c$ then,

$$P_{d(mw)} = \frac{(y_c + L) - (y_w - l)}{2L} = \frac{L + l - y_w + y_c}{2L} \quad (\text{B4})$$

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Table 1. Parameters used in simulation and analytical models for computations for heterogeneous aquifer conditions.

Case	Simulation model						Analytical model	
	longitudinal dispersivity, α_L (m)	transverse dispersivity, α_T (m)	mean of Y , μ_Y	variance of Y , σ_Y^2	correlation length, λ (m)	mean velocity, v (m/day)	longitudinal macrodispersivity, A_L (m)	transverse macrodispersivity, A_T (m)
Case 1a	0.1	0.01	2.3	0.2	15	0.04	3.1	0.01325
Case 1b	0.1	0.01	2.3	0.4	15	0.04	6.1	0.0165
Case 1c	0.1	0.01	2.3	1.0	15	0.04	15.1	0.02625
Case 1d	0.1	0.01	2.3	1.5	15	0.04	22.6	0.034375
Case 2a	0.5	0.05	2.3	0.2	15	0.04	3.5	0.06625
Case 2b	0.5	0.05	2.3	0.4	15	0.04	6.5	0.0825
Case 2c	0.5	0.05	2.3	1.0	15	0.04	15.5	0.13125
Case 2d	0.5	0.05	2.3	1.5	15	0.04	23	0.171875

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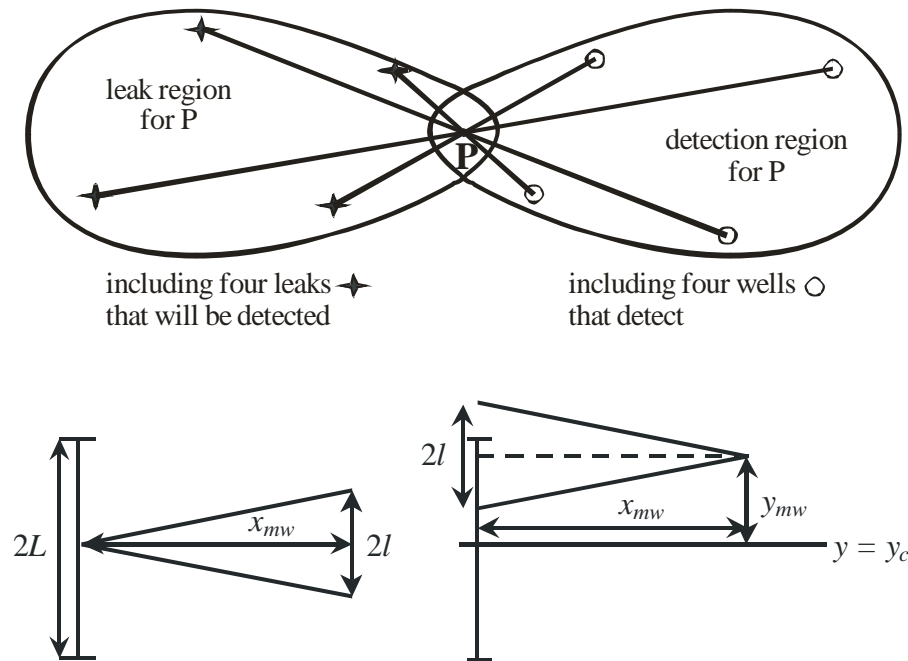


Fig. 1. Depiction of detect and leak regions.

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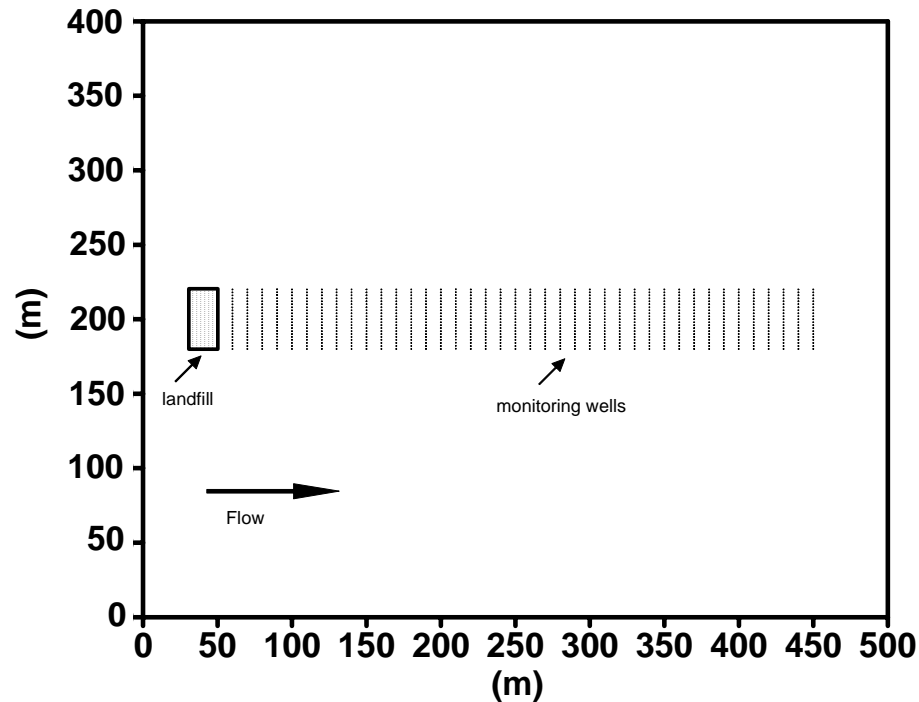


Fig. 2. Dimensions and components of the example with 840 monitoring well locations.

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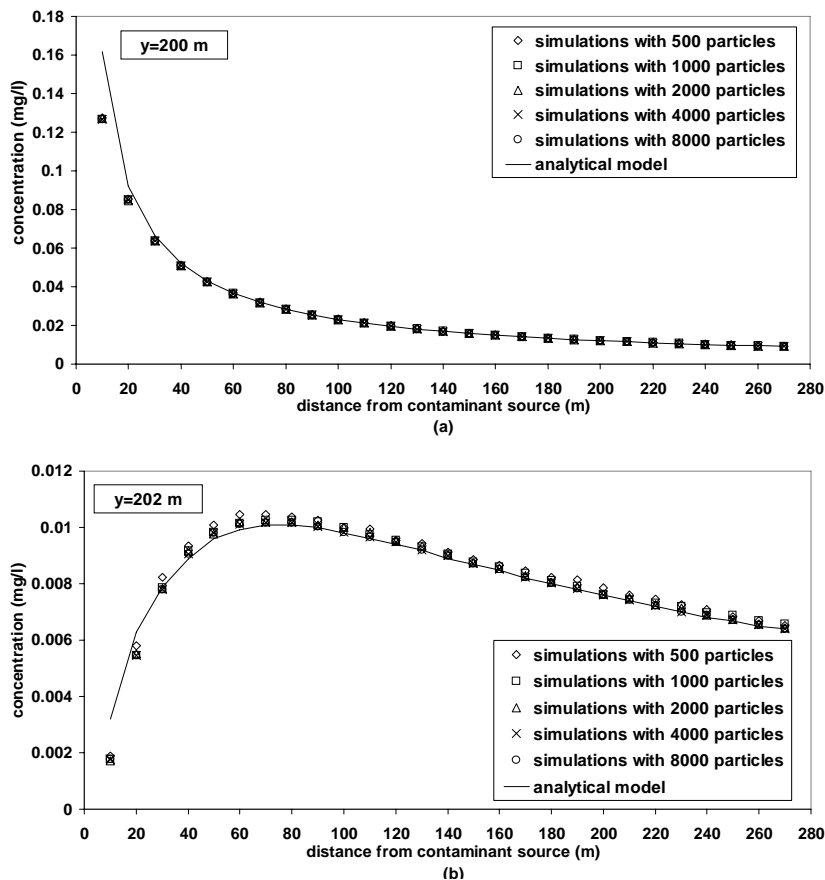


Fig. 3. Comparison of simulation and analytical model of a contaminant plume originated from an instantaneous leak ($y=200$ m) in the homogeneous case for $\alpha_L=0.1$ m, $\alpha_T=0.01$ m for longitudinal sections along (a) $y=200$ m, (b) $y=202$ m and (c) $y=204$ m.

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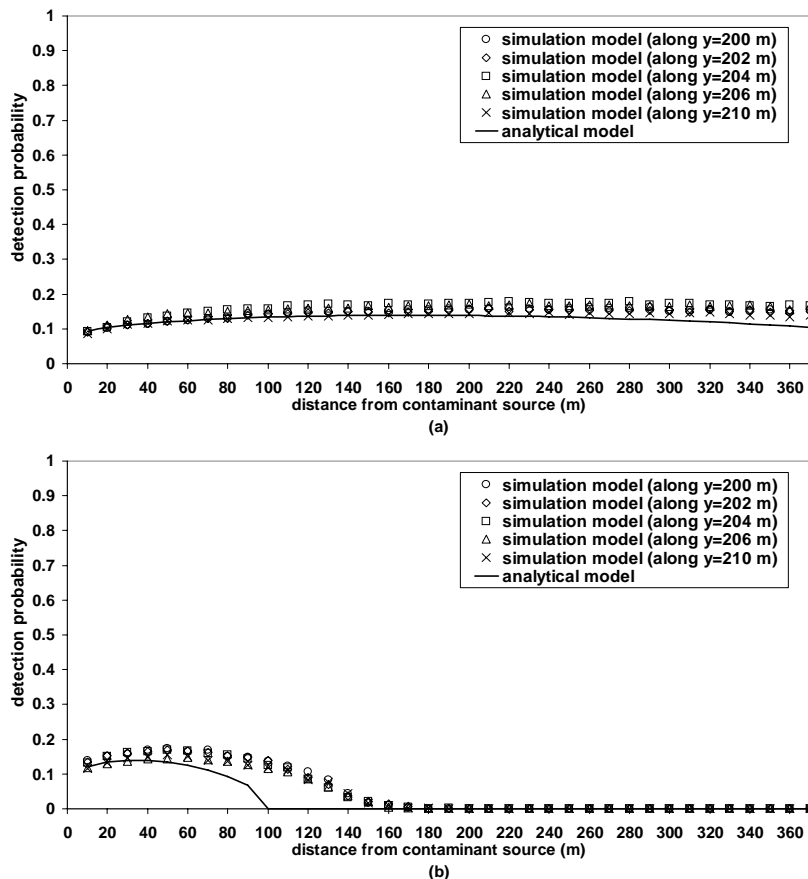


Fig. 4. Comparison of detection probability values at selected well locations computed by simulation and analytical models for an instantaneous leak in the homogeneous case **(a)** $\alpha_L=0.1$ m, $\alpha_T=0.01$ m and **(b)** $\alpha_L=0.5$ m, $\alpha_T=0.05$ m.

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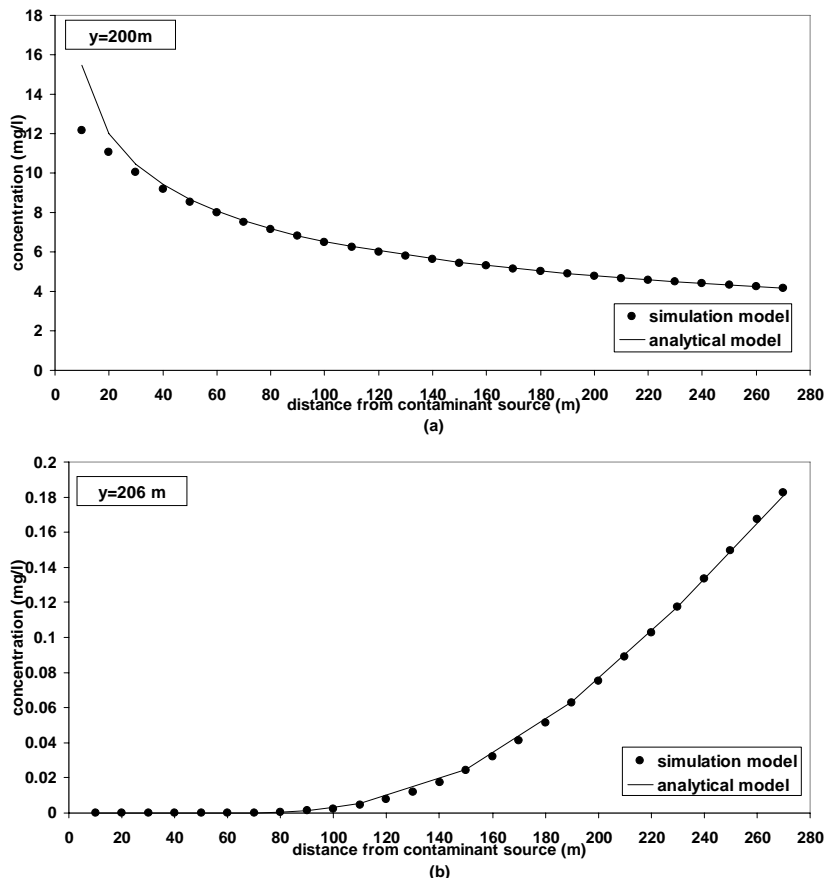


Fig. 5. Comparison of simulation and analytical model of a contaminant plume originated from a continuous leak in the homogeneous case with $\alpha_L=0.1\text{ m}$, $\alpha_T=0.01\text{ m}$ for longitudinal sections along (a) $y=200\text{ m}$ and (b) $y=206\text{ m}$.

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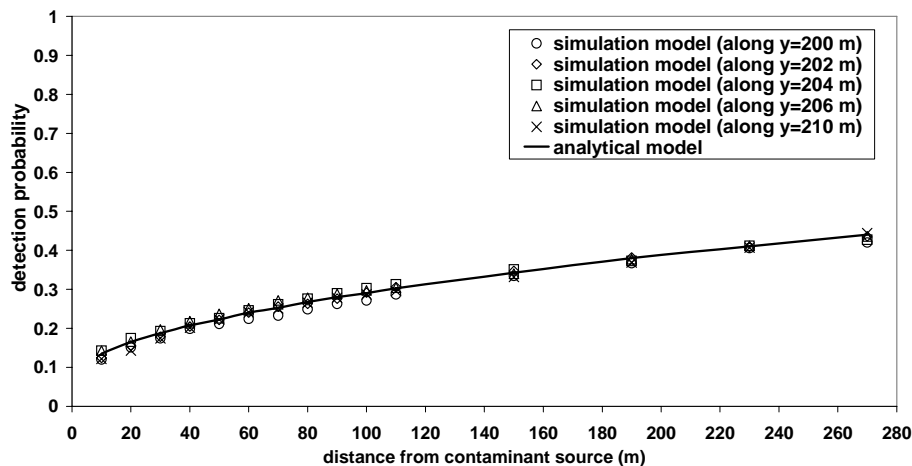


Fig. 6. Comparison of detection probability values at selected well locations computed by simulation and analytical models for a continuous leak in the homogeneous case ($\alpha_L=0.1$ m, $\alpha_T=0.01$ m).

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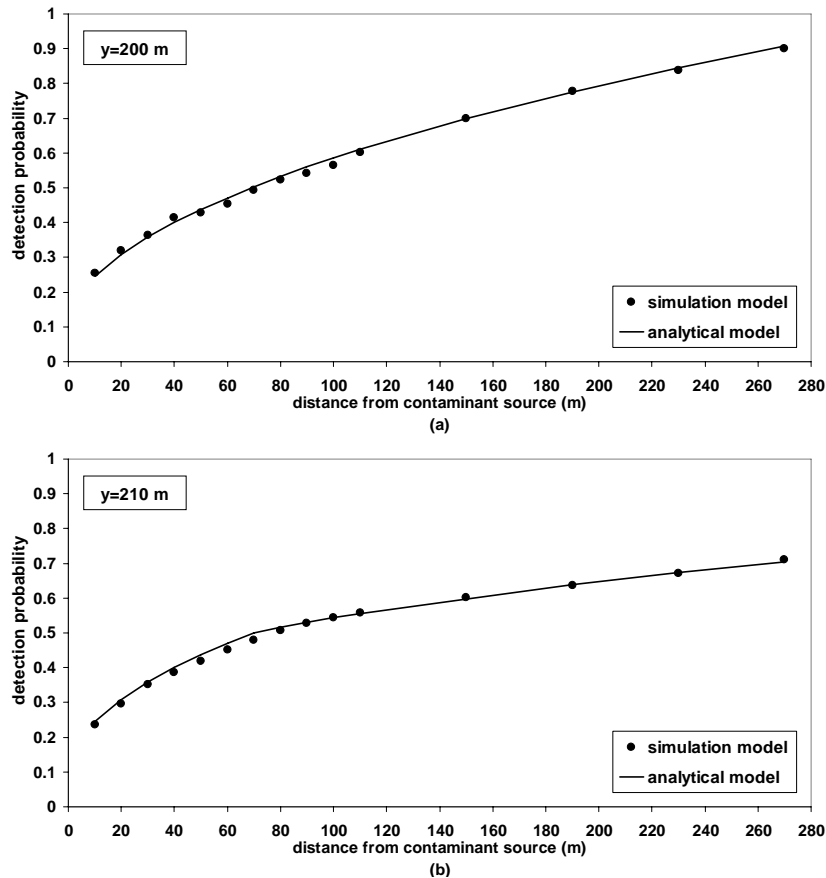


Fig. 7. Comparison of detection probability values at selected well locations computed by simulation and analytical models for a continuous leak in the homogeneous case ($\alpha_L=0.5$ m, $\alpha_T=0.05$ m) **(a)** along $y=200$ m and **(b)** along $y=210$ m.

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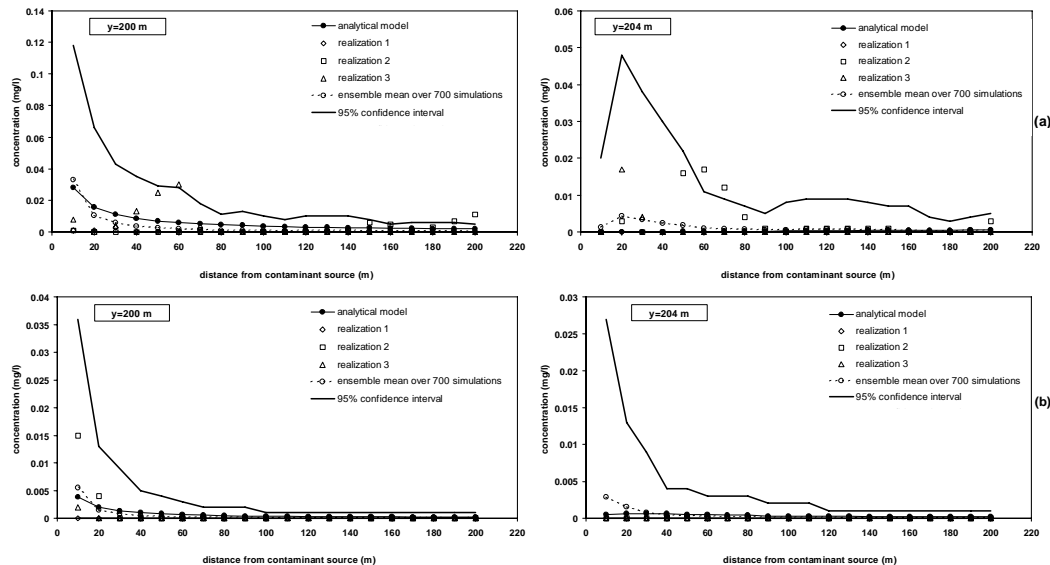


Fig. 8. Comparison of simulation and analytical model of a contaminant plume originated from an instantaneous leak ($y=200$ m) in the heterogeneous case for longitudinal sections along $y=200$ m (left column) and $y=204$ m (right column) **(a)** Case 1a **(b)** Case 2d.

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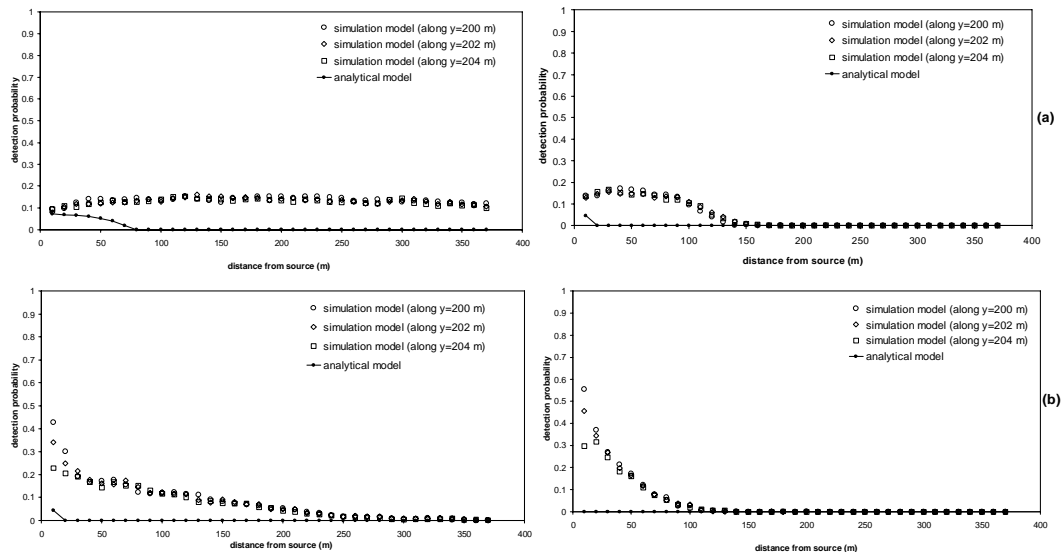


Fig. 9. Comparison of detection probability values at selected well locations computed by simulation and analytical models for an instantaneous leak in the heterogeneous case **(a)** Case 1a and Case 2a, **(b)** Case 1d and Case 2d.

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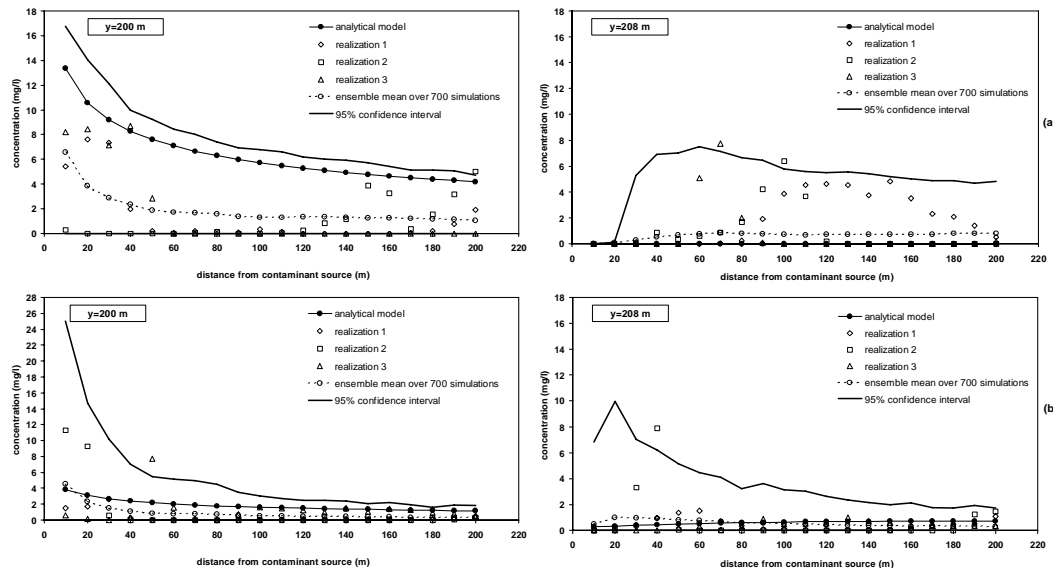


Fig. 10. Simulation and analytical model comparison of a contaminant plume originated from a continuous leak ($y=200$ m) in the heterogeneous case for longitudinal sections along $y=200$ m (left column) and $y=204$ m (right column) **(a)** Case 1a, and **(b)** Case 2d.

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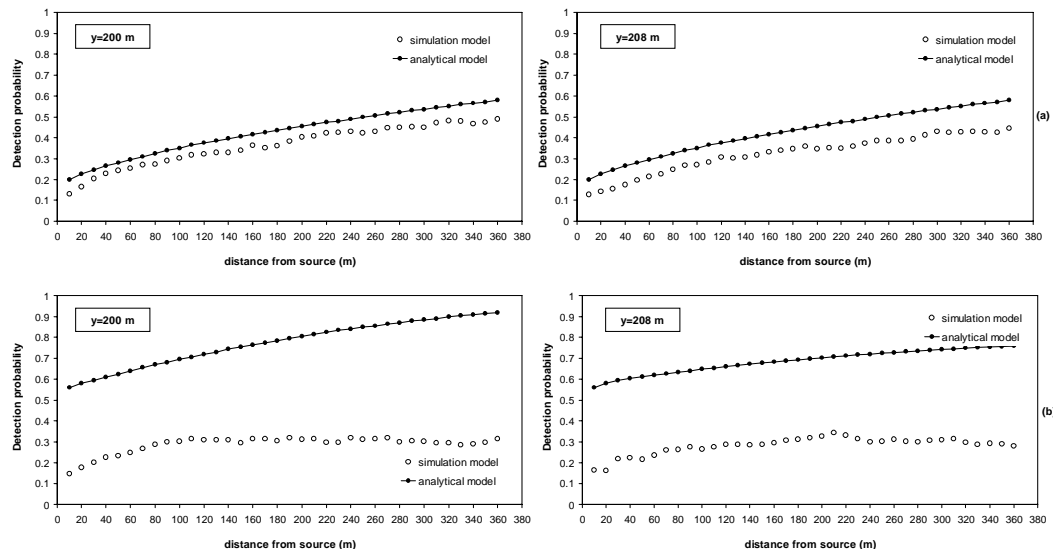


Fig. 11. Comparison of detection probability values at selected well locations computed by simulation and analytical models for continuous leak in a heterogeneous medium along $y=200$ m (left column) and $y=208$ m (right column) **(a)** Case 1a, and **(b)** Case 1d.

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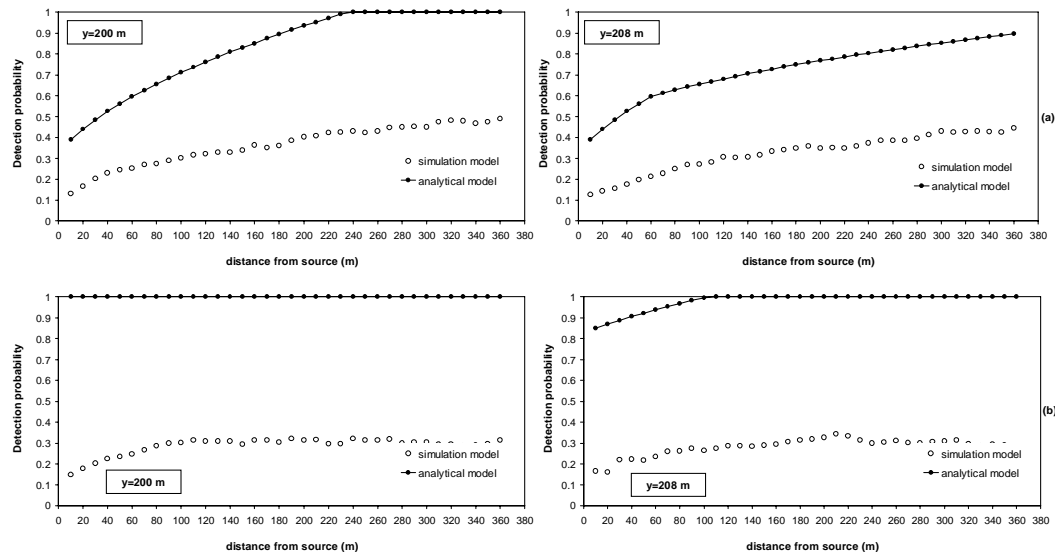


Fig. 12. Comparison of detection probability values at selected well locations computed by simulation and analytical models for continuous leak in a heterogeneous medium along $y=200$ m (left column) and $y=208$ m (right column) **(a)** Case 2a, and **(b)** Case 2d.

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